

# Sharp phase transitions in a small frustrated network of trapped ion spins

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Sharp quantum phase transitions typically require a large system with many particles. Here we show that for a frustrated fully-connected Ising spin network represented by trapped atomic ions, the competition between different spin orders leads to rich phase transitions whose sharpness scales exponentially with the number of spins. This unusual finite-size scaling behavior opens up the possibility of observing sharp quantum phase transitions in a system of just a few trapped ion spins.

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Quantum simulators are motivated by the promise of gaining insight into many-body quantum systems such as high- $T_C$  superconductors or complex arrangements of interacting spins. Cold atomic systems form a promising platform for quantum simulation, as the interactions between particles can be under great control. A good example is a collection of trapped and laser-cooled atomic ions, each representing an effective spin that can be made to interact with all the others by modulating the Coulomb interaction between ions. By applying spin-dependent optical dipole forces it has been shown that a crystal of ions provides an ideal platform to simulate intractable interacting spin models [1, 2]. Following this proposal, recent experiments have simulated quantum magnetism with a few ions [3–6]. For three or more ions, the long-range coupling between the spins can provide frustrated interaction patterns or competition between various spin orders and interesting quantum phase diagrams [5, 6]. However, the observation of a quantum phase transition typically requires a large system with many particles, as the width (sharpness) of a quantum phase transition usually scales with  $1/N$ , the inverse of the number of particles [7]. With such slow finite-size scaling laws, small networks of trapped ions realized in current experiments ( $N \lesssim 20$ ) are not expected to exhibit sharp transitions between distinct quantum phases.

In this paper, we show the surprising result that sharp phase transitions can indeed be observed with just a few atomic ions. This is due to unusual finite size scaling laws in this frustrated spin network, where the sharpness of some phase transitions scales exponentially instead of linearly with  $1/N$ . By controlling a single experimental parameter that determines the pattern of spin-spin couplings between the ions, we show that the expected ground state emerges from a delicate compromise between the couplings. Frustration in the spin network leads to a variety of spin orders, with the number of distinct phases increasing rapidly with the number of ions. We construct the complete phase diagram for small spin networks realizable with the current technology. The sharp phase transition is characterized in detail with an explanation of its unusual finite-size scaling behavior.

We consider a small crystal of ions confined in a

one-dimensional harmonic trap. The spin states of the ions are represented by two internal states, referred as  $|\uparrow\rangle$  and  $|\downarrow\rangle$ , and the effective spin-spin interaction between the ions is induced with off-resonant bichromatic laser beams [1, 3–5]. The ion-laser coupling Hamiltonian, written in the rotating frame, has the form  $H = \sum_n [\hbar\Omega \cos(\delta k x_n + \mu t) \sigma_n^z + B \sigma_n^x]$  [8], where  $\Omega$  is a Raman Rabi frequency,  $\delta k$  is the wave vector difference between the two Raman beams (which is assumed to be along the radial direction  $\hat{x}$ ),  $\mu$  is the beatnote or detuning between the two laser beams,  $\sigma_n^z$  and  $\sigma_n^x$  are Pauli matrices describing the spin of the  $n$ th ion, and  $B$  is an effective magnetic field induced by radiation that coherently flips the spins. In the rotating frame, the radial coordinate  $x_n$  is expanded in terms of the transverse phonon modes  $a_k$  as  $x_n = \sum_k b_n^k \sqrt{\hbar/(2m\omega_k)} (a_k^\dagger e^{i\omega_k t} + a_k e^{-i\omega_k t})$ , where  $m$  is the atomic mass,  $\omega_k$  is the eigenfrequency of the  $k$ th normal mode of the ion crystal, and  $b_n^k$  is the eigenmode transformation matrix. We use transverse phonon modes because they can more easily be scaled up to large systems [5, 9]. Under the Lamb-Dicke criterion  $\eta_{n,k} \equiv b_n^k \delta k \sqrt{\hbar/(2m\omega_k)} \ll 1$ , the Hamiltonian  $H$  is simplified to  $H = -\hbar\Omega \sum_{n,k} \eta_{n,k} \sin(\mu t) \sigma_n^z (a_k^\dagger e^{i\omega_k t} + a_k e^{-i\omega_k t}) + B \sum_n \sigma_n^x$ .

If we assume that the laser detuning  $\mu$  is not resonant with any phonon mode with the condition  $|\omega_k - \mu| \gg \eta_{n,k}\Omega$  satisfied for all  $n$  modes  $k$ , the probability of exciting any phonon mode  $|\Omega \eta_{n,k} b_n^k / 2 (\omega_k - \mu)|^2$  is negligible. We can therefore adiabatically eliminate the phonon modes and arrive at the following effective spin-spin coupling Hamiltonian [6, 10]

$$H_s = \sum_{m,n} J_{mn} \sigma_m^z \sigma_n^z + B \sum_n \sigma_n^x, \quad (1)$$

where the coefficients

$$J_{mn} = \frac{(\hbar\Omega\delta k)^2}{2m} \sum_k \frac{b_m^k b_n^k}{\mu^2 - \omega_k^2}. \quad (2)$$

This Ising Hamiltonian is a pillar of many-body physics, and its properties have been exhaustively studied under various conditions [7]. For instance, the ground

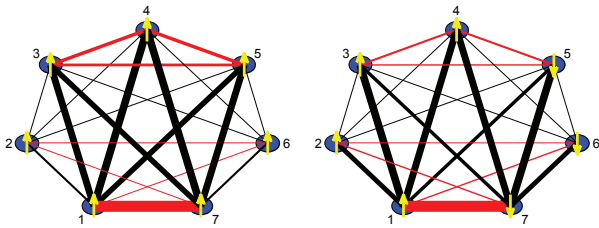


Figure 1: (Color online) Illustration of spin orders in two frustrated Ising networks with competing long-range interaction for  $N = 7$  ions. *Left panel*: Ferromagnetic (FM) order with detuning  $\tilde{\mu} = 5.1$ ; *Right panel*: Kink order with  $\tilde{\mu} = 5.3$ . The thickness of the edge in the graph represents the strength of each coupling. Positive (AFM) spin couplings are indicated in red, while negative (FM) couplings are indicated in black.

state of the Ising Hamiltonian is well understood when the coupling coefficients  $J_{mn}$  are uniform, or nonzero only for nearest neighbors. However, here we have an extended Ising network where the coupling coefficients  $J_{mn}$  are inhomogeneous (both in magnitude and sign) and extend over long range [11]. The strong competition among these interaction terms (even with  $B = 0$ ) will generally lead to highly frustrated ground states where individual bonds are compromised in order to reach a global energy minimum. For arbitrary coupling coefficients  $J_{mn}$ , the Hamiltonian (1) generally belongs to the complexity class of NP-complete problems [12], meaning that calculating attributes such as the system ground state becomes intractable when the system size is scaled up.

We consider the case where the coupling coefficients  $J_{mn}$  are controlled by a single experimental parameter, the laser detuning  $\mu$  [4–6]. To determine  $J_{mn}$  from any detuning  $\mu$  with the formula (2), we first need the normal mode transformation matrix  $b_n^k$ . This is obtained by finding the equilibrium positions for a given number of ions in a harmonic trap and then diagonalizing the Coulomb interaction Hamiltonian expanded about the ions' equilibrium positions. With a single control parameter  $\mu$ , we are not able to program arbitrary coupling coefficients  $J_{mn}$ . However, the interaction pattern is sufficiently complex to allow frustrated ground state configurations and rich phase transitions. To illustrate this we show in Fig. 1 a coupling pattern for  $N = 7$  ions and its associated ground state spin configuration for  $B = 0$ . The coupling pattern is represented by a graph where the color and the thickness of each edge represents respectively the sign (ferromagnetic or antiferromagnetic) and the magnitude of the coupling. In Fig. 1(a), we find a ferromagnetically ordered ground state with all the spins pointing to the same direction. However, in this ferromagnetic state, some of the bonds, such as the strong antiferromagnetic bond between the ions 1 and 7, are compromised, and due to this frustration, the ground-state spin configuration is very sensitive to the strength of the coupling. If we adjust the detuning  $\mu$  by a small fraction of the trap frequency, the ferromagnetic bonds of the ion pairs (1, 5) and (3, 7) are

slightly weakened (see Fig. 1(b)) and the antiferromagnetic bond (1, 7) dominates and flips the spin direction of the entire left (or right) half of the ion crystal. This is a phase transition from ferromagnetic order to a “kink” order, with a kink in the spin direction between the 4th and 5th ions counting from either the left or the right side.

To show the rich phase diagram for this system, in Fig. 2(a) we list all different spin phases at  $B = 0$  for a small Ising network with 3, 5, 7 and 9 ions. For an odd number of ions, the phase diagram is more interesting and features a larger variety of spin orders, because the left-right reflection symmetry in a linear ion crystal can be spontaneously broken. In Fig. 2, for convenience, we denote the laser detuning  $\mu$  with a re-scaled dimensionless parameter  $\tilde{\mu}$  by labeling the phonon-mode eigen-frequencies (from lowest to highest) with integers (from 1 to  $N$  for an  $N$ -ion crystal) and using a linear scaling between two integers to denote detuning located between the corresponding two modes. For instance, in this notation  $\tilde{\mu} = 2.75$  means the physical detuning  $\mu = \omega_2 + 0.75(\omega_3 - \omega_2)$ . Each phase is characterized by a spin order (denoted with a binary string where 0 and 1 correspond to  $\uparrow$  and  $\downarrow$  spin respectively) which gives one of the ground state spin configurations. The Ising Hamiltonian (1) features a reflection symmetry and an intrinsic  $Z_2$  symmetry with respect to a global spin flip. The spin order breaks the Ising symmetry, so each phase is at least two-fold degenerate. If the spin order also breaks the reflection symmetry, the corresponding ground state is 4-fold degenerate. For instance, for the phase denoted by the spin order 01001, the four degenerate ground states are  $|\downarrow\uparrow\downarrow\downarrow\uparrow\rangle$ ,  $|\uparrow\downarrow\uparrow\uparrow\downarrow\rangle$ ,  $|\uparrow\downarrow\downarrow\uparrow\downarrow\rangle$ , and  $|\downarrow\uparrow\uparrow\downarrow\uparrow\rangle$ . When the re-scaled detuning  $\tilde{\mu}$  crosses an integer (a phonon mode), the spin order changes as expected, but this is not a conventional phase transition as the parameters  $J_{mn}$  change discontinuously in the Hamiltonian (1). However, when  $\tilde{\mu}$  varies within two adjacent integers, all the parameters  $J_{mn}$  are analytic functions of  $\tilde{\mu}$ , yet the spin order can still change abruptly, signaling a phase transition. The frequency of this type of inter-mode phase transition increases rapidly with the ion number: there is one such transition for a three-ion chain and 12 such transitions in a nine-ion crystal. Another notable feature from Fig. 2(a) is that there is typically no phase transition when  $\tilde{\mu}$  varies from an even mode ( $2k$ ) to an odd mode ( $2k + 1$ ,  $k = 0, 1, \dots, (N - 1)/2$ ). In such regions, the spin order has a reflection symmetry. This suggests that a spin order with reflection symmetry may be more stable in energy and does not easily yield to other spin configurations. This observation is consistent with the fact that for an even number of ions, there are much fewer inter-mode phase transitions, as the spin order in these cases has a reflection symmetry.

As we add a transverse  $B$  field to the Hamiltonian, the spins will gradually become polarized along the  $x$ -direction along  $B$ . In Fig. 2(b), we plot the average polarization  $\langle \sum_n \sigma_n^x \rangle / N$  as a function of the field  $B$  (in the unit of the average  $J_{mn}$  defined by  $\bar{J} \equiv$

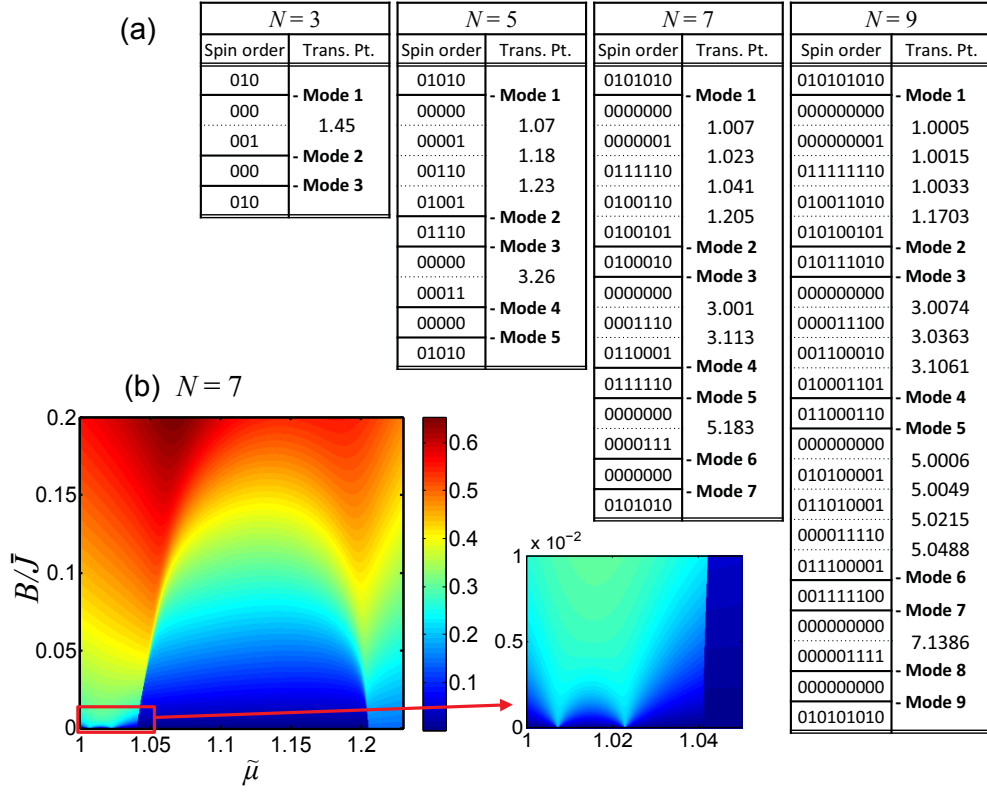


Figure 2: (Color online) (a) Ground-state phase diagram at  $B = 0$  characterized by the corresponding spin orders for  $N = 3, 5, 7, 9$  ions. The transition point is denoted by the re-scaled detuning  $\tilde{\mu}$ . (b) Average polarization  $\langle \sum_n \sigma_n^x \rangle / N$  for  $N = 7$  ions at finite fields  $B$ . The right figure is a closeup near the critical point.

$\sqrt{\sum_{m \neq n} |J_{mn}|^2 / [N(N-1)]}$  for  $N = 7$  ions in a small region of the detuning  $\tilde{\mu}$ . We find that the system is easily polarized if it lies at the critical point between two different spin orders given by the Ising couplings. But near the center of a spin phase, the spin order is more robust and can persist under a finite  $B$ , eventually yielding to the polarized phase as  $B$  increases through the Ising-type transition (which becomes a broad crossover for this finite system).

With  $B = 0$ , the transition between different spin orders is sharp as it is characterized by a level crossing for the ground state of the Hamiltonian (1). When we turn on a finite  $B$  field, the system shows only avoided level crossings in its ground state, and we expect that the sharp phase transition at  $B = 0$  to be replaced by a broad crossover for this small system, similar to the Ising-type of transition discussed above. Interestingly, this is not always the case. Even at a finite  $B$ , some transitions remain very sharp in this small system, and the sharpness increases exponentially with the number of particles. This provides an unusual finite-size scaling behavior, distinctively different than the polynomial finite-size scaling of the transition width that one typically sees in conventional phase transitions [7]. (For instance, the conventional Ising transition displays a linear scaling law [7].) To characterize this unusual finite-size scaling behavior,

we look at a particular example: for  $N$  ions, there is a unique spin phase transition in the region with detuning  $N - 2 < \tilde{\mu} < N - 1$  when  $N$  is odd. A schematic phase diagram for this region is shown in Fig. 3(a). At  $B = 0$ , we have a ferromagnetic phase on the left side which is doubly degenerated and a kink phase on the right side which is 4-fold degenerate. At finite  $B$ , these two spin orders remain robust in a range of  $B$ , before eventually yielding to a polarized phase for a large  $B$  field through a crossover. The transition between the ferromagnetic and the kink phases remain sharp for a finite  $B$ , and this sharpness increases rapidly with the ion number, as one can see from Fig. 3(b) and 3(c). With a moderate increase of the ion number from 5 to 9, the transition between the ferromagnetic and the kink phase becomes almost infinitely sharp. It is also interesting to note that the transition line between these two phases has a slope with the  $B$  axis, so one can cross this phase transition by tuning either the detuning  $\tilde{\mu}$  or the field  $B$ .

We have characterized the transition width between the ferromagnetic phase and the kink phase, and find this transition width indeed shrinks exponentially with the number of ions. To see this, we show the four lowest levels across this phase transition when we tune either  $\tilde{\mu}$  or  $B$  (see Fig. 4a). While the lowest state is a smooth function of  $\tilde{\mu}$  at a finite  $B$ , the second and third states feature

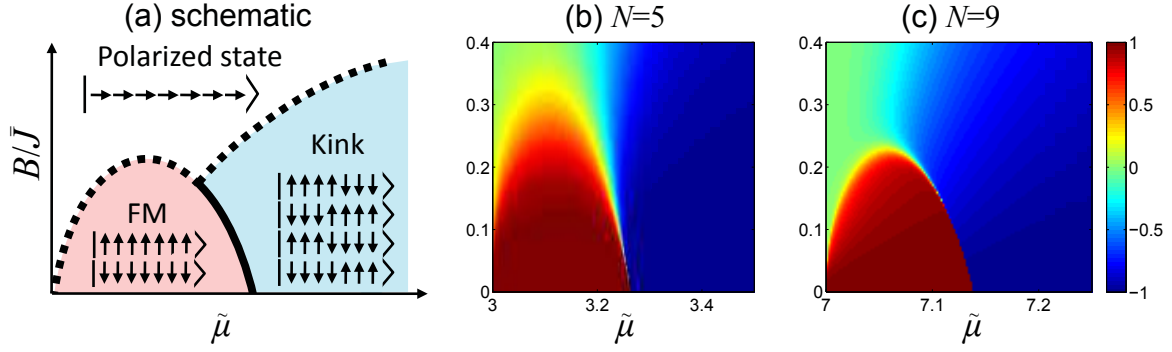


Figure 3: (Color online) (a) The schematic phase diagrams for odd numbers of ions in the region with detuning  $N-2 < \tilde{\mu} < N-1$ . For a small number of ions, the solid line represents a sharp transition, whereas the dashed lines represent a continuous crossover to the polarized state. (b,c) The calculated theoretical phase diagrams for (b)  $N = 5$  and (c)  $N = 9$  ions. Color shows the order parameter defined by  $P_{FM} - P_K$ , where  $P_{FM}$  and  $P_K$  are the projection probabilities of the ground state of the system to the Hilbert subspace with the ferromagnetic and the kink orders, respectively (the basis-vectors of the corresponding subspaces are indicated in Fig. (a)).

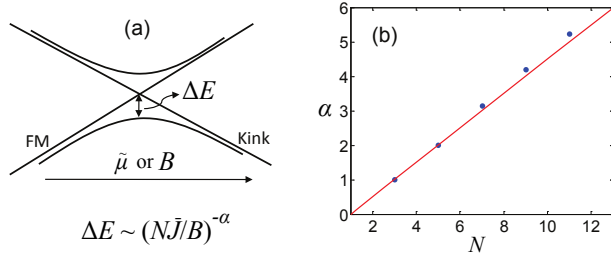


Figure 4: (a) The structure of the lowest four energy levels around the sharp ferromagnetic-kink phase transition. The two lowest states have a ferromagnetic (kink) order on the left (right) side. The transition width  $W$  is proportional to the energy gap  $\Delta E$ , and  $\Delta E$  is fitted by an exponential. (b) The exponent  $\alpha$  is a function of the ion number  $N$ , where the solid line is a linear fit  $\alpha \simeq (N-1)/2$ .

a level crossing. From Fig. 4a, the transition width  $W$  is proportional to the energy gap  $\Delta E$ . We calculate the energy gap  $\Delta E$  as a function of the ion number  $N$ , and find it is well fit by  $\Delta E \propto (B/N\bar{J})^\alpha$  for  $B \ll N\bar{J}$ , where the exponent  $\alpha$  has a roughly linear dependence with  $N$  as shown in Fig. 4b and can be fit by  $\alpha \simeq (N-1)/2$ . This formula shows that the energy gap  $\Delta E$ , and thus also the transition width  $W$ , shrinks exponentially with

the ion number, which explains why the transition is so sharp for a small system. The exponential shrinking of the energy gap  $\Delta E$  can be intuitively understood as follows: when  $B \ll N\bar{J}$  we can treat the term  $B \sum_n \sigma_n^x$  as a perturbation in the Hamiltonian (1). For each application of  $B \sum_n \sigma_n^x$ , we can only flip the direction of one spin. As the ferromagnetic state and the kink state have  $(N-1)/2$  spins taking opposite directions, the two states need to be connected through  $(N-1)/2$ th order perturbation, and thus the energy gap is proportional to  $(B/N\bar{J})^{(N-1)/2}$ .

In summary, we have shown that laser induced magnetic coupling between trapped ions realizes a frustrated Ising spin network with competing long range interactions, giving rise to rich phase diagrams for the ground state. Some of the phase transitions in this system are characterized by a unusual finite size scaling, where the transition width scales down exponentially with the number of ions. This exponential finite size scaling leads to sharp phase transitions for a small system even with just a few ions, as one can realize now in the lab.

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